Bryce

NATIONAL BUREAU OF STANDARDS REPORT

1643

I. B. M. EXPERIMENTS WITH ACCELERATED

GRADIENT METHODS FOR LINEAR EQUATIONS

by

A. I. Forsythe

and

G. E. Forsythe

National Bureau of Standards, Los Angeles

NBS

U. S. DEPARTMENT OF COMMERCE
NATIONAL BUREAU OF STANDARDS

U. S. DEPARTMENT OF COMMERCE
Charles Sawyer, Secretary

NATIONAL BUREAU OF STANDARDS
A. V. Astin, Acting Director

THE NATIONAL BUREAU OF STANDARDS

The scope of activities of the National Bureau of Standards is suggested in the following listing of the divisions and sections engaged in technical work. In general, each section is engaged in specialized research, development, and engineering in the field indicated by its title. A brief description of the activities, and of the resultant reports and publications, appears on the inside of the back cover of this report.

1. ELECTRICITY. Resistance Measurements. Inductance and Capacitance. Electrical Instruments. Magnetic Measurements. Electrochemistry.
2. OPTICS AND METROLOGY. Photometry and Colorimetry. Optical Instruments. Photographic Technology. Length. Gage.
3. HEAT AND POWER. Temperature Measurements. Thermodynamics. Cryogenics. Engines and Lubrication. Engine Fuels.
4. ATOMIC AND RADIATION PHYSICS. Spectroscopy. Radiometry. Mass Spectrometry. Physical Electronics. Electron Physics. Atomic Physics. Neutron Measurements. Nuclear Physics. Radioactivity. X-Rays. Betatron. Nucleonic Instrumentation. Radiological Equipment. Atomic Energy Commission Instruments Branch.
5. CHEMISTRY. Organic Coatings. Surface Chemistry. Organic Chemistry. Analytical Chemistry. Inorganic Chemistry. Electrodeposition. Gas Chemistry. Physical Chemistry. Thermochemistry. Spectrochemistry. Pure Substances.
6. MECHANICS. Sound. Mechanical Instruments. Aerodynamics. Engineering Mechanics. Hydraulics. Mass. Capacity, Density, and Fluid Meters.
7. ORGANIC AND FIBROUS MATERIALS. Rubber. Textiles. Paper. Leather. Testing and Specifications. Organic Plastics. Dental Research.
8. METALLURGY. Thermal Metallurgy. Chemical Metallurgy. Mechanical Metallurgy. Corrosion.
9. MINERAL PRODUCTS. Porcelain and Pottery. Glass. Refractories. Enameled Metals. Building Stone. Concreting Materials. Constitution and Microstructure. Chemistry of Mineral Products.
10. BUILDING TECHNOLOGY. Structural Engineering. Fire Protection. Heating and Air Conditioning. Exterior and Interior Coverings. Codes and Specifications.
11. APPLIED MATHEMATICS. Numerical Analysis. Computation. Statistical Engineering. Machine Development.
12. ELECTRONICS. Engineering Electronics. Electron Tubes. Electronic Computers. Electronic Instrumentation.
13. ORDNANCE DEVELOPMENT. Mechanical Research and Development. Electromechanical Fuzes. Technical Services. Missile Fuzing Research. Missile Fuzing Development. Projectile Fuzes. Ordnance Components. Ordnance Tests. Ordnance Research.
14. RADIO PROPAGATION. Upper Atmosphere Research. Ionospheric Research. Regular Propagation Services. Frequency Utilization Research. Tropospheric Propagation Research. High Frequency Standards. Microwave Standards.
15. MISSILE DEVELOPMENT. Missile Engineering. Missile Dynamics. Missile Intelligence. Missile Instrumentation. Technical Services. Combustion.

NBS PROJECT

1101-21-5102

March 10 1952

NBS REPORT

1643

I. B. M. EXPERIMENTS WITH ACCELERATED GRADIENT METHODS FOR LINEAR EQUATIONS*

by

A. I. Forsythe

and

G. E. Forsythe

National Bureau of Standards, Los Angeles

NBS

PREPRINT

*The preparation of this paper was sponsored (in part) by the Office of Naval Research, USN

NBS 1643
3-10-52
PREPRINT

I. B. M. Experiments with Accelerated Gradient Methods for Linear Equations *

by

A. I. Forsythe

and

G. E. Forsythe

National Bureau of Standards, Los Angeles

I. SUMMARY

Various gradient (steepest descent) methods for solving systems of linear equations have been discussed by Cauchy [2], Temple [12], Kantorovich [9], and others. The method usually discussed, the optimum gradient method (explained in section II), ordinarily converges too slowly for practical use. Under the general leadership of Professor Magnus Hestenes at the Institute for Numerical Analysis several methods have been studied for speeding up the gradient method.

A class of modified gradient methods, in which one overshoots or undershoots the optimum point, is presented in [7]. In [11] Stein presents numerical experiments with the matrix B_0 used below, showing that consistently undershooting ("almost optimum" gradient method) provides a self-accelerating procedure. Motzkin and one

*The preparation of this paper was sponsored (in part) by the Office of Naval Research.

of us propose [5] an acceleration step to be inserted occasionally into the optimum gradient method. (In section II we give Hestenes' interpretation of this device as a minimization in two dimensions.) The purpose of the I. B. M. experiments now reported was to test the latter acceleration procedure. Incidental to this, we obtained additional data on the optimum, almost optimum, and other gradient methods.

A survey of the formulas used is given in section II, and the numerical experiments are summarized in section III. In section IV we study these data in some detail. Section V contains the references referred to in the text by numbers in square brackets.

In brief, it is our conclusion that for two test matrices of order six, the acceleration speeds the optimum gradient method up by a factor of from 7 to 18, and makes the optimum method possibly useful. The almost optimum gradient method is something like half as fast as our accelerated procedure (on the basis of two test matrices) but - and this is very important for machine work - the almost optimum gradient method is simpler to code. The more recently developed methods of Hestenes and Stiefel [8] now appear to offer much faster convergence at a modest increase in complexity.

II. SUMMARY OF THE THEORY

For simplicity we deal with the field of real numbers. Let A be an n-by-n matrix, not singular, and let x, b denote n-rowed column vectors. We are interested in finding the solution $A^{-1}b$ of the system

(1) $$Ax = b \quad .$$

Let T denote transposition of a matrix. The positive definite matrix $B = A^T A$ and the vector $c = A^T b$ will frequently be used. The length $|y|$ of a column vector y will be defined by $|y|^2 = y^T y$. We use θ to denote the zero vector.

Let $f(x) = |Ax - b|^2$ measure the deviation of any vector x from the solution $A^{-1}b$.

One can verify that

(2) $$f(x) = x^T Bx - 2x^T c + |b|^2 \quad .$$

Suppose x is a given approximation to $A^{-1}b$, and let d be a given direction. As an improvement of x we may select the vector $y(\alpha) = x - \alpha d$ for which $f[y(\alpha)]$ assumes its minimum as a function of the real variable α. The corresponding value of α will be called γ.

To obtain a formula for γ, we first find from (2) that

(3) $$f[y(\alpha)] = f(x) + \alpha^2 d^T Bd - 2\alpha d^T (Bx - c) \quad .$$

Introducing the abbreviation

(4) $$\xi = Bx - c \quad ,$$

we find from (3) that

(5) $$\gamma = d^T \xi / d^T Bd \quad .$$

In the optimum gradient method for solving (1), suggested by

Cauchy [2] and analyzed by Temple [12], Kantorovich [9], Hestenes and Karush [6] (for the eigenvalue problem), and others, one selects any x_0, and then obtains each x_{k+1} from x_k as follows: For each k, one picks d_k to be $\frac{1}{2}$ grad $f(x_k) = Bx_k - c = \xi_k$, and takes

$$x_{k+1} = x_k - \gamma_k \xi_k , \qquad \xi_k = Bx_k - c \quad , \tag{6}$$

where, by (5),

$$\gamma_k = \xi_k^T \xi_k / \xi_k^T \xi_k \quad . \tag{7}$$

Kantorovich showed on pp. 144, 154 of [9] that in the optimum gradient method

$$\max_{x_{k-1}} \frac{f(x_k)}{f(x_{k-1})} = \left(\frac{\lambda_n - \lambda_1}{\lambda_n + \lambda_1}\right)^2 = \mu^2 < 1 \quad , \tag{8}$$

where λ_n and λ_1 are, respectively, the largest and least of the (necessarily positive) eigenvalues of B. It follows that

$$|Ax_k - b| \leq |Ax_0 - b|\mu^k \to 0, \qquad \text{as } k \to \infty \quad , \tag{9}$$

so that the method converges. Our experience suggests that the inequality in (9) is usually nearly an equality; see section IV. Since μ is commonly near* 1, the optimum gradient method is

---

*If all the elements of A have the same normal distribution, it results from p. 59 of [1] that the "probable" value of μ is "about" $1 - 4m^{-2}$. (The precise meaning of this is not stated in [1].)

usually too slowly convergent for practical use. In section III we give examples of the optimum gradient method.

Many proposals have been made to speed up the process. In [7] Hestenes and Stein describe a family of modified gradient methods in which one changes formula (6) to read

$$x_{k+1} = x_k - \beta \gamma_k \xi_k , \quad \xi_k = Bx_k - c , \tag{10}$$

where β is a fixed factor in the range $0 < \beta < 2$, and prove the convergence. For β near 0.9 (called the "almost optimum" gradient method) the evidence in Stein [11] suggests that the convergence is much faster than for the optimum gradient method ($\beta = 1$). In section III we summarize these data, and give more of our own.

Other proposed accelerations of the gradient method involve getting x_{k+1} by minimizing $f(x)$ in the p-dimensional linear subspace $x = x_{k-p} - \alpha_1 \xi_{k-p} - \alpha_2 B \xi_{k-p} - \cdots - \alpha_p B^{p-1} \xi_{k-p}$ ($1 < p \leq n$; α_i real and arbitrary). (This is equivalent to minimizing $f(x)$ in the linear p-space containing x_{k-p}, x_{k-p+1}, ..., and x_k.) Kantorovich [9] suggests use of $p = 2$. Karush [10] considers the analogous process with a general p in solving the eigenvalue problem. In [8] Hestenes and Stiefel give an iterative method which effectively can give p any value up to n. (When $p = n$ the method is an exact solution of (1).) Motzkin and one of us propose [5] an acceleration step which Professor Hestenes has shown to be equivalent to taking $p = 2$. We now describe this.

It is a conjecture (stated in [5]; proved for $n = 3$ in [4]; seemingly confirmed in the present experiments) that

$$(11)\quad \left\{\begin{array}{l}\underline{\text{in the optimum gradient method the error vector}}\\ x_k - A^{-1}b\ \underline{\text{is asymptotically a linear combination}}\\ \underline{\text{of the eigenvectors}}\ u_1,\ u_n\ \underline{\text{of}}\ B\ \underline{\text{belonging to the}}\\ \underline{\text{largest}}\ (\lambda_n)\ \underline{\text{and least}}\ (\lambda_1)\ \underline{\text{eigenvalues of}}\ B.\end{array}\right.$$

(If there are eigenvectors of B orthogonal to $x_0 - A^{-1}b$, one disregards the corresponding eigenvalues in determining λ_1 and λ_n.) When this asymptotic relationship holds for a given x_0, the sequence $\{x_k - A^{-1}b\}$ behaves asymptotically as though it were in the 2-plane π containing u_1 and u_n. But

$$(12)\quad \left\{\begin{array}{l}\underline{\text{if one carries out the optimum gradient process in}}\\ \underline{\text{any 2-plane}\ \pi'}, \underline{\text{the vectors}}\ x_k - A^{-1}b\ \underline{\text{alternate}}\\ \underline{\text{between two directions in}\ \pi'}, \underline{\text{and, for each}}\ k,\ \underline{\text{the}}\\ \underline{\text{line joining}}\ x_{k-2}\ \underline{\text{and}}\ x_k\ \underline{\text{passes through}}\ A^{-1}b.\end{array}\right.$$

It is therefore the proposal of [5] that the optimum gradient method occasionally be interrupted by determining the $x_{k+1} = \alpha x_k + (1 - \alpha)x_{k-2}$ which minimizes $f[x(\alpha)]$. If the acceleration procedure occurs after m steps, the computing procedure is to set $x = x_m$ and $d = x_{m-2} - x_m$ in (4) and (5), and the acceleration formulas are:

$$(13)\quad \left\{\begin{array}{ll}d_m = x_{m-2} - x_m & ,\\ \zeta_m = Bx_m - c & ,\\ \gamma_m = d_m^T \zeta_m / d_m^T B d_m & ,\\ x_{m+1} = x_m - \gamma_m d_m & .\end{array}\right.$$

It is Professor Hestenes' observation that

$$(14)\quad \begin{cases} \underline{\text{the } x_{k+1} \text{ of any acceleration step is the vector in}} \\ \underline{\text{the two-dimensional subspace}}\ x(\alpha_1, \alpha_2) = x_{k-2} \\ -\alpha_1 \xi_{k-2} - \alpha_2 B \xi_{k-2}\ \underline{\text{which minimizes}}\ f[x(\alpha_1, \alpha_2)] \\ \underline{\text{with respect to}}\ \alpha_1\ \underline{\text{and}}\ \alpha_2 . \end{cases}$$

Since, in using the optimum gradient method numerically, one is already set up to carry out the types of operations involved, the procedure (13) may be preferable to a more direct method for carrying out the above two-dimensional minimization. (The extension of this idea to the use of n successive one-dimensional steps to minimize $f(x)$ in n dimensions is at the basis of the algorithm in [8].) In section III will be found reports of numerical experiments with the acceleration step. Various numbers of optimum gradient steps have been tried between accelerations.

We also report insertion of the acceleration step (13) into the modified gradient method (10) for $\beta = 1.1$. In this case Professor Hestenes' interpretation does not hold.

Of the various statements made above, the only ones which require proof are (12) and (14).

To prove (12) we may assume without loss of generality that $b = \theta$. It then suffices to show that x_2 is parallel to x_0. The loci $f(x) =$ constant are similar ellipses in π. Let t_0 be the tangent at x_0 to the ellipse through x_0. Then the gradient ξ_0 at x_0 is orthogonal to t_0. Since ξ_0 is also the tangent t_1 at x_1 to the ellipse through x_1, ξ_0 is also orthogonal to ξ_1, the gradient at x_1. Being both orthogonal to ξ_0, the lines ξ_1 and t_0 are parallel.

Since ξ_1 is a tangent at x_2 to the ellipse through x_2, x_2 is parallel to x_0, as was to be proved.

To prove 14, we note that (12) implies that the acceleration step will locate the common center of the ellipses formed by the intersection of the surfaces $f(x)$ = constant with the plane through x_{k-2}, x_{k-1}, and x_k. It therefore suffices to prove that this plane is actually the plane $x_{k-2} - \alpha_1 \xi_{k-2} - \alpha_2 B\xi_{k-2}$ (α_i arbitrary). But $\xi_{k-1} = Bx_{k-1} - c = B(x_{k-2} - \gamma_{k-2}\xi_{k-2}) - c = \xi_{k-2} - \gamma_{k-2} B\xi_{k-2}$. Then $x_k = x_{k-1} - \gamma_{k-1}\xi_{k-1} = x_{k-2} - (\gamma_{k-2} + \gamma_{k-1})\xi_{k-2} - \gamma_{k-2}\gamma_{k-1} B\xi_{k-2}$. Hence the non-collinear points x_k, x_{k-1}, and x_{k-2} are all in the plane of $x_{k-2} - \alpha_1 \xi_{k-2} - \alpha_2 B\xi_{k-2}$, and (14) is proved.

When the conjectured asymptotic behavior (11) occurs for a given x_0, we saw above that $x_k - A^{-1}b$ asymptotically approaches θ while alternating between two directions L, L' in the plane π. Here L, L' are related by the fact that their conjugate* directions with respect to the ellipses $f(x)$ = constant in π are orthogonal. When $n = 3$ the proof in [4] of (11) shows that, when x_0 has a projection on each eigenvector of B, not all pairs L, L' are eligible to be asymptotic directions of $x_k - A^{-1}b$. Roughly speaking, the eligible directions L, L' are those for which $f(x_k)/ f(x_{k-1})$ (which has one value for both L and L') is sufficiently near its maximum value μ^2; see (8).

---

* Two directions are conjugate with respect to an ellipse if they are the directions of a radius (from the center) and a tangent at the same point.

For each direction L of $x - A^{-1}b$ there is a ratio $\rho = \rho(L)$ of $f(x)$ to $|x - A^{-1}b|^2$; here $\rho(L)$ is commonly unequal to $\rho(L')$. We see that

$$(15) \qquad \rho(L) = \frac{|Ax - b|^2}{|x - A^{-1}b|^2} = \frac{(x - A^{-1}b)^T B(x - A^{-1}b)}{|x - A^{-1}b|^2} \quad .$$

Thus $\rho(L)$ is the Rayleigh quotient of the error vector $x - A^{-1}b$. We therefore have

$$(16) \qquad \lambda_1 \leq \rho(L) \leq \lambda_n ;$$

see p. 26 of [3], for example. From the foregoing it follows that, whenever the conjectured asymptotic behavior (11) of x_k holds, $|x_k - A^{-1} b|$ goes to zero in such a manner that the ratio $|x_k - A^{-1}b|/|x_{k-1} - A^{-1}b|$ will alternately approach the two limits $\mu\rho(L)/\rho(L')$, $\mu\rho(L')/\rho(L)$. Only for the special case when $\rho(L) = \rho(L')$ (meaning that L, L' have symmetric positions with respect to the major axis of the ellipses) will these limits be equal.

It is instructive to study the modified gradient process (10) analytically in two dimensions. Some of the characteristic behavior of the runs reported in section III occurs — the instability of $f(x_k)/f(x_{k-1})$ for β slightly less than 1, and the approach of $f(x_k)/f(x_{k-1})$ to μ^2 for most x_0 when $1 < \beta \leq \beta_0 < 2$. This study has been started by one of us with Motzkin [unpublished], and will not be reproduced here.

III. EXPERIMENTS AND TABLES

The several methods described in section II were tried out with two essentially different systems of order six on the IBM Card-Programmed Calculator of the Institute for Numerical Analysis. The order six is the largest for which an ordinary gradient step could be handled with the internal storage of the machine used; for these exploratory experiments it was thought better to spend as little time as possible using external storage. (Even so, our acceleration steps required external storage.) The coefficients of the first system, $Ax = b$, were obtained from a table of random digits simulating a population of equally distributed integers $-99, -98, \ldots, 0, \ldots, +99$. We obtained

$$A = \begin{bmatrix} -14 & 55 & 61 & 40 & 3 & 47 \\ 27 & -34 & 17 & -89 & -78 & 39 \\ 13 & 92 & -63 & 26 & 15 & -86 \\ -23 & 86 & 30 & 95 & -80 & -76 \\ 12 & 52 & 17 & 61 & -34 & 42 \\ -70 & -64 & 42 & 47 & 23 & 28 \end{bmatrix},$$

$$b = [-93, \quad -96, \quad -71, \quad 26, \quad -69, \quad 71]^T.$$

In the methods reported here A and b do not explicitly enter the calculations, but only $B = A^TA$ and $c = A^Tb$. For the above matrix the latter are given a subscript 0; for scaling purposes B_0 was then multiplied by 10^{-5}, and c_0 by 10^{-6}.

$$B_0 = \begin{bmatrix} .06667 & .02634 & -.04640 & -.07368 & -.02131 & -.00431 \\ .02634 & .26841 & -.02243 & .15952 & -.05923 & -.12797 \\ -.04640 & -.02243 & .10932 & .05150 & -.04100 & .08558 \\ -.07368 & .15952 & .05150 & .25152 & -.01141 & -.07169 \\ -.02131 & -.05923 & -.04100 & -.01141 & .14403 & .01105 \\ -.00431 & -.12797 & .08558 & -.07169 & .01105 & .19450 \end{bmatrix},$$

$$c_0 = [-.008609, -.014279, -.000243, +.004576, +.008043, -.004895]^T .$$

Our first experiments were carried out with B_0, c_0, in order to study the machine procedure on a matrix without zeros. These B_0 and c_0 were also used by Stein [11], who calls them A and b.

The gradient methods are invariant under translations and rotations of the space, as long as the operations are carried out exactly. The machine operations are much faster with a diagonal matrix, and the behavior of x_k is more easily studied in the coordinate system of the eigenvectors of B_0. Accordingly the positive definite matrix B_0 was reduced* to its diagonal form $B_1 = S B_0 S^T$, where S is an orthogonal matrix. At the same time c_0 was replaced by $c_1 = \theta$, the zero-vector, so that the solution became θ. (Probably in practice the round-off errors with B_1, c_1 are less than with B_0, c_0, but these errors are not studied here.)

We have

*Mr. R. M. Hayes determined B_1 and S on the Card-Programmed Calculator.

$$B_1 = \begin{bmatrix} .00268704\ (=\lambda_1) & & & & & \bigcirc \\ & .01581310\ (=\lambda_2) & & & & \\ & & .08234830\ (=\lambda_3) & & & \\ & & & .17590130\ (=\lambda_4) & & \\ & \bigcirc & & & .25946632\ (=\lambda_5) & \\ & & & & & .49823436\ (=\lambda_6) \end{bmatrix},$$

$$c_1 = [0, \quad 0, \quad 0, \quad 0, \quad 0, \quad 0]^T.$$

The ratio $P = \lambda_6/\lambda_1 \doteq 200$ of the eigenvalues of B_0 and B_1 was noted in section II to be intimately related to the speed of convergence of the optimum gradient method; indeed, from (8),

$$\mu = (P - 1)\ (P + 1)^{-1} \doteq 1 - 2P^{-2}.$$

To get data from a system for which convergence was likely to be faster, we selected a diagonal matrix B_2 with $P = 36$.* The other eigenvalues λ_i were selected at random from tables simulating a rectangular distribution of $\log \lambda_i$ on the interval $\log \lambda_1 \leq \log \lambda_i \leq \log \lambda_6$. We obtained

$$B_2 = \begin{bmatrix} .01 & & & & & \bigcirc \\ & .02 & & & & \\ & & .11 & & & \\ & & & .15 & & \\ & \bigcirc & & & .22 & \\ & & & & & .36 \end{bmatrix},$$

$$c_2 = [0, \quad 0, \quad 0, \quad 0, \quad 0, \quad 0,]^T.$$

---

*Under the hypothesis of our footnote, page 4 above, the "probable" value of P is "about" n^2.

For each matrix we used various modifications of the gradient method, and began with various initial vectors x_0. A summary of the experiments run is contained in Table 2. On the Card-Programmed Calculator we used a ten-digit board with fixed decimal point, designed by Dr. Everett C. Yowell of the Institute for Numerical Analysis. Under the supervision of one of us the experiments were run by Messrs. Thomas D. Lakin, William O. Paine, Jr., and Albert H. Rosenthal.

The data were checked in two ways: (i) the $\{f(x_k)\}$ were scanned for reasonableness; (ii) the experiments with matrices B_0 and B_1 were run twice. Since check (ii) seldom indicated an error which had not been suspected from check (i), it was decided to get extra data for matrix B_2 by omitting check (ii). These data therefore have a higher probability of error than those for matrices B_0 and B_1, but we hope that they are essentially correct.

In Table 1 we show the detailed progress of one run.* The matrix and initial vector are the same (in a different coordinate system) as those reported by Stein [11], and the table may be compared with his Table I. The run chosen consists of 8 optimum gradient steps ($\beta = 1.0$), alternated with one acceleration. Since $\beta = 1.0$, it results from (14) that this is equivalent to 6 minimizations of $f[x(\alpha)]$ on the line $x = x_k - \alpha \xi_k$, followed by one minimization of $f[x(\alpha_1, \alpha_2)]$ in the 2-plane $x = x_k - \alpha_1 \xi_k - \alpha_2 B \xi_k$; and repeat. If we used a machine with sufficient internal storage, the amount of effort in each cycle would be reasonably equivalent to 9 of the optimum gradient steps.

*The run is identified by an arrow in Table 2.

TABLE 1

One of Our Accelerated Runs

k	$10^2 f(x_k)$	$r(k-1,k) = f(x_k)/f(x_{k-1})$
0	.33360 3	
1	.11925 6	.3575
2	8538 1	.7159
3	6999 2	.8198
4	6230 4	.8902
5	5779 8	.9277
6	5490 5	.9499
7	5263 8	.9587
8	5075 5	.9642
9	4150 5	.8178
10	3431 4	.8267
11	3341 0	.9737
12	3258 1	.9752
13	3179 6	.9759
14	3103 7	.9761
15	3030 1	.9763
16	2958 3	.9763
17	2888 3	.9763
18	178 10	.0617
19	62 250	.3495
20	36 544	.5871
21	27 418	.7503
22	23 845	.8697
23	21 457	.8999
24	19 557	.9114
25	17 950	.9178
26	16 551	.9221
27	7 1404	.4314
28	6 0682	.8498
29	5 7512	.9478
30	5 5369	.9627
31	5 3678	.9695
32	5 2465	.9774
33	5 1293	.9777
34	5 0148	.9777
35	4 9030	.9777
36	5055 7	.0103
37	3085 3	.6103
38	2230 8	.7230
39	1736 2	.7783
40	1445 8	.8327
41	1267 0	.8763
42	1114 1	.8793
43	980 01	.8796
44	.00000 00 862 25	.8798

k	$10^2 f(x_k)$	$r(k-1,k) = f(x_k)/f(x_{k-1})$
45	.00000 00011 072	.0128
46	35833	.0324
47	30050	.8386
48	28349	.9434
49	26827	.9463
50	25449	.9486
51	24199	.9509
52	23060	.9529
53	22021	.9549
54	11206	.5089
55	5767 7	.5147
56	5382 4	.9332
57	5104 0	.9483
58	4880 1	.9561
59	4690 0	.9610
60	4520 2	.9638
61	4365 5	.9658
62	4222 2	.9672
63	2420 9	.5734
64	1956 0	.8080
65	1779 9	.9100
66	1684 4	.9463
67	1601 4	.9507
68	1527 8	.9540
69	1459 0	.9550
70	1394 6	.9559
71	1334 0	.9565
72	343 23	.2573
73	88 906	.2590
74	82 480	.9277
75	80 370	.9744
76	78 402	.9755
77	76 509	.9758
78	74 670	.9760
79	72 880	.9760
80	.00000 00000 00071 138	.9761

k	$10^2 f(x_k)$	$r(k-1,k) = f(x_k)/f(x_{k-1})$
81	.00000 00000 00007 1757	.1009
82	3 4982	.4875
83	2 3839	.6815
84	1 9269	.8083
85	1 7004	.8824
86	1 5681	.9222
87	1 4526	.9263
88	1 3506	.9298
89	1 2597	.9327
90	52499	.4168
91	44791	.8532
92	41313	.9224
93	39336	.9521
94	37650	.9571
95	36157	.9603
96	34726	.9604
97	33354	.9605
98	32038	.9605
99	1068 1	.0333
100	36 674	.0343
101	32 874	.8964
102	32 156	.9782
103	31 458	.9783
104	30 775	.9783
105	30 108	.9783
106	29 455	.9783
107	28 817	.9783
108	34263	.0119
109	12630	.3686
110	9811 6	.7768
111	7884 4	.8036
112	6344 9	.8047
113	5111 7	.8056
114	4118 6	.8057
115	3318 7	.8058
116	2674 3	.8058
117	4 3660	.0016
118	.00000 00000 00000 00000 00002 8111	.6439

This type of run showed the fastest convergence of $f(x_k)$ to 0; detailed comparisons with other runs will be found in Table 2 and section IV below.

In Table 1 each heavy horizontal rule indicates an acceleration step. The small discrepancies from the data in [11] result from round-off errors in rotating the coordinate system.

To save space and bring out the important features of the data, the other runs are presented here only in summary form (Table 2). The columns of that table are now described.

Column 1: Here we give the matrix $B = A^T A$, and vector $c = A^T b$.

Column 2: Here we give the initial column vector, x_0. We use the following abbreviations:

$$\theta = (\ 0, \quad 0, \quad 0, \quad 0, \quad 0, \quad 0\ )^T$$

$$x_0^{(1)} = (\ .1, \quad .1, \quad -.1, \quad -.1, \quad .1, \quad -.1,\ )^T$$

$$x_0^{(2)} = (-.1, \quad -.1, \quad .1, \quad .1, \quad .1, \quad .1\ )^T$$

$$x_0^{(3)} = (\ .4595, \quad .0790, \quad .1200, \quad .0880, \quad .0150, \quad .0113)^T$$

$$x_0^{(4)} = (\ .005, \quad .005, \quad .005, \quad .005, \quad .005, \quad .01\ )^T$$

$$x_0^{(5)} = (\ .01, \quad .01, \quad .01, \quad .01, \quad .01, \quad .01\ )^T$$

$$x_0^{(6)} = (\ .1, \quad .1, \quad .1, \quad .1, \quad .1, \quad .1\ )^T$$

$$x_0^{(7)} = (\ .05, \quad .05, \quad .05, \quad .05, \quad .05, \quad .1\ )^T$$

$$x_0^{(8)} = (\ .1, \quad .05, \quad .05, \quad .05, \quad .05, \quad .05\ )^T$$

Most of these vectors were chosen without any special significance, to see how the methods varied with different starts. The vector θ is a reasonable start with the non-homogeneous problem with B_0, c_0. The vector $x_0^{(3)}$ in the coordinate system of B_1, θ is identical with θ in the coordinate system of B_0, c_0.

Column 3: β is defined in (10).

Column 4: For all β, a straight run is an iteration of the step in formula (10).

For $\beta \neq 2$, the term "m steps and accelerate" means that m steps of type (10), resulting in $x_0, \ldots, x_{m-2}, x_{m-1}, x_m$, are alternated with a minimization of $f(x)$ for x along the line joining x_{m-2} and x_m, according to (13).

For $\beta = 2$ a special acceleration was performed: After getting the points $x_0, x_1, \ldots, x_7, x_8$, one optimum gradient ($\beta = 1$) step was taken from the point $x = \frac{1}{2}(x_7 + x_8)$. Then 8 more steps followed with $\beta = 2$; etc.

Column 5: In getting the total number, called s, of steps of a run, each acceleration is counted as one step.

Column 6: The number $r(k_1, k_2)$ measures the mean proportionate reduction in $f(x_k)$ per step, for k between k_1 and k_2, where $k_1 < k_2$. It is defined by the relation

$$(17) \qquad r(k_1, k_2) = \left(\frac{f(x_{k_2})}{f(x_{k_1})} \right)^{\frac{1}{k_2 - k_1}}$$

We may interpret $r(k_1, k_2)$ as the geometric mean of the $k_2 - k_1$ ratios $\left\{ f(x_i)/f(x_{i-1}) \right\}$ $(i = k_1 + 1, k_1 + 2, \ldots, k_2)$.

It seems to us that for appropriate choice of k_1, k_2, $r(k_1, k_2)$ is a useful index of the average speed of the iterative process for solving the system $Ax = b$. For the modified gradient processes with $0 < \beta < 2$, one always has $0 \leq r(k_1, k_2) < 1$. One must remember, however, that the time of convergence of an iteration varies linearly with $\log(1/r)$, not with r; see (14) and Table 4.

The quantity $r(0, s)$ would measure the average reduction in $f(x)$ from the beginning x_0 to the end x_s of a run. Since in some runs a substantial portion of the reduction from $f(x_0)$ to $f(x_s)$ occurs in the first few steps, where x_k has not yet settled down (see Table 1), the quantity $r(0, s)$ gives a deceptively high impression of the speed of an iteration. To avoid this initial effect, we selected $k_1 = 5$, and accordingly have tabulated $r(5, s)$ in column 6 as a measure of the mean speed of the process over the major portion of the run.

<u>Column 7</u>: In certain of the processes the quantity $r(k-1, k) = f(x_{k-1})/f(x_k)$ settles down and appears to approach a limit. (The conjecture (11) would imply that, for all x_0, $f(x_{k-1})/f(x_k)$ approaches a limit in the optimum gradient process.) Since this limit would be a measure of the ultimate speed of the process, we give the last value, $r(s-1, s) = f(x_{s-1})/f(x_s)$, in column 7. In other processes, where the ratio $f(x_{k-1})/f(x_k)$ does not settle down, we make no entry.

For comparison with Table 2, we present in Table 3 a summary of Stein's runs [11] in the same form.

TABLE 2

Summary of Our Runs

(1) MATRIX	(2) START	(3) β	(4) METHOD	(5) NO. OF STEPS (s)	(6) r(5,s)	(7) r(s-1,s)
B_0, c_0	θ	1.0	4 Steps and accelerate	76	.8226	
B_0, c_0	θ	1.0	7 " " "	65	.8002	
"	"	"	8 " " "	44	.7552	
"	"	"	9 " " "	49	.8334	
"	"	"	12 " " "	80	.8295	
"	$x_0^{(1)}$	"	8 " " "	83	.8379	
"	$x_0^{(2)}$	"	8 " " "	54	.7717	
B_1, θ	$x_0^{(3)}$	2.0	Straight Run	77	1.0000	
"	"	1.1	" "	119	.9775	.9786
"	"	1.0	" "	70	.9733	.9748
"	"	.9	" "	87	.8204	
"	"	2.0	8 Steps and accelerate	78	.8749	
"	"	1.1	" " "	79	.7873	
"	"	1.0	" " "	119	.6245	
"	$x_0^{(4)}$	.9	Straight Run	75	.8150	
"	"	1.0	" "	53	.9421	.9758
"	$x_0^{(5)}$	.9	" "	85	.8310	
"	"	1.0	" "	40	.9293	.9693
B_2, θ	$x_0^{(6)}$	1.0	8 Steps and accelerate	55	.4566	
"	"	"	Straight Run	74	.8836	.8939
"	"	.9	" "	73	.6530	
B_2, θ	$x_0^{(7)}$	1.0	8 Steps and accelerate	117	.4738	
"	"	1.0	Straight Run	69	.8809	.8917
"	"	.9	" "	71	.7117	
B_2, θ	$x_0^{(8)}$	1.0	8 Steps and accelerate	123	.4373	
"	"	"	Straight Run	73	.8903	.8938
"	"	.9	" "	71	.6333	

Note: B_1 is similar to B_0. B_1, θ with $x_0^{(3)}$ is same problem as B_0, c_0 with θ.

TABLE 3

Summary of Stein's Runs

(1) MATRIX	(2) START	(3) β	(4) METHOD	(5) NO. STEPS	(6) r(5,s)	(7) r(s-1,s)
B_o, c_o	θ	.1	Straight Runs	30	.9334	
"	"	.3	"	30	.9509	
"	"	.6	"	30	.9339	
"	"	.8	"	30	.8685	
"	"	.85	"	30	.9156	
"	"	.9	"	30	.8065	
"	"	.95	"	30	.9454	
"	"	1.0	"	30	.9702	.9742
"	"	1.1	"	30	.9737	.9779
"	"	1.3	"	30	.9739	.9779
"	"	1.6	"	30	.9728	.9779
"	"	1.9	"	30	.9385	.9744

It may be useful occasionally to transform $r = r(k_1, k_2)$ to a unit which is proportional to the time spent in an iteration. Let $K = K(r)$ be the number of steps needed to reduce $|Ax_k - b|$ by one decimal place; i.e., to one-tenth of its value, when $f(x_{k-1})/f(x_k)$ has the mean value r. Since $f(x_k) = |Ax_k - b|^2$, we find K(r) from the relation

$$r^{K(r)} = 10^{-2} ,$$

whence

$$K(r) = \frac{2}{\log_{10}(1/r)} . \tag{14}$$

In Table 4 we give K(r) for some values of r. Note that a small variation in r near 1 makes a large difference in K(r); the quantity K is an approximate measure of the time required to solve a system.

IV. STUDY OF THE DATA

The first question we faced was: at what intervals should the acceleration step (13) best be applied to the optimum gradient method (6)? There seem to be two possibilities. (i) Some property of the sequence $\{x_k\}$ might indicate when it was ready to be accelerated — for example, the property of having x_{k-3}, x_{k-2}, x_{k-1}, x_k almost in a 2-plane. To simplify the I.B.M. procedure this was not tried. (ii) The acceleration step could be inserted after each m steps. The latter procedure was adopted, and we needed to select a preferred value of m.

TABLE 4

Iterative Steps Per 1-Decimal Reduction of $|Ax - b|$

r	K(r)
.01	1.0
.1	2.0
.2	2.9
.3	3.8
.4	5.1
.5	6.6
.6	9.0
.7	13.0
.8	20.6
.85	33.0
.90	43.7
.91	48.8
.92	55.3
.93	63.5
.94	74.4
.95	89.8
.96	113
.97	164
.98	227
.985	305
.990	458
.991	509
.992	574
.993	656
.994	765
.995	919
.996	1149
.997	1533
.998	2300
.999	4603

For the matrix B_0 we made several tests designed to choose m. In one, starting always with a vector near the x_{36} of Table 1, we repeatedly ran 12 optimum gradient steps and an acceleration step. These thirteen steps were performed in 10 different ways, viz., with the acceleration step following the 2nd, 3rd, ..., or 11th optimum gradient step. The results of the test (not shown in this paper) were that one got to the least f(x) in these thirteen steps when the acceleration was taken as late as possible. This fact by itself suggests taking a large value of m. On the other hand, use of a large m means that relatively fewer accelerations can be taken in a run of a given number of steps. Since the main reduction in f(x) comes in the accelerations, one wants as many such steps as possible.

The balance between these opposing factors determines the best value for m. For the matrix B_0 we tried out m = 4, 7, 8, 9, and 12. Study of the values of r(5,s) for the runs with B_0 at the start of Table 2 indicates that (for $x_0 = \theta$) m = 8 is best, while m = 7 is next best.

It is probable that the optimal value of m depends on the value of the initial vector x_0. We suspect, however, that the variation of m with x_0 is commonly slight, because each acceleration is a complicated transformation which effectively produces a new initial vector. Thus each single run is the average of a number of different starts. With matrices B_0 and B_2 the procedure with m = 8 was run for more than one start x_0. The variation in r(5,s) is not great; see Table 2. That m depends materially on the matrix B and its order m is not questioned; it would be an interesting experiment to study the dependence on these factors.

Having accepted $m = 8$ as the best value for the matrix B_0 (and for the similar matrix B_1), we retained $m = 8$ for the matrix B_2, but we do not claim it to be optimal.

Table 1 shows a run of 118 steps with matrix B_1, using $m = 8$ and starting with the vector $x_0^{(3)}$, which corresponds to the start θ for B_0 used above and in [11]. The table of values of $f(x_k)$ and their ratios shows what a complicated process we are dealing with. By a cycle we refer to a block of eight optimum gradient steps followed by one acceleration. The cycles vary greatly in their success in reducing $f(x_k)$. When the optimum gradient steps within a cycle bring $x_k - A^{-1}b$ nearly into the plane π defined in section 2, then the following acceleration brings $f(x_{k+1})$ to a value much less than $f(x_k)$. The efficiency of the next following cycles varies within wide bounds, apparently according to rather subtle properties of the vector $x_{k+1} - A^{-1}b$. Thus the progress of the error vector to zero is irregular, and the values of r in Table 1 are certainly not predictable. Part of the reason for this is that, as can be shown, the asymptotic behavior of the direction vectors $(x_k - A^{-1}b)/|x_k - A^{-1}b|$ is exceedingly sensitive to a change in the initial vector x_0.

Nevertheless - and this is the important practical consideration - in the accelerated procedure x_k was able to progress rapidly toward the solution $A^{-1}b$. For the matrix B_1, the average reduction $r(5,119)$ in $f(x)$ was .6245 (Table 2), representing a speed of convergence 18 times as fast as that of the optimum gradient method, for which $r(86,87) = .9748$. (i.e. $(.9748)^{18} \doteq .6245$.) For the matrix B_2, the

corresponding figures for starts $x_0^{(6)}$, $x_0^{(7)}$, $x_0^{(8)}$ were .4566 and .8939, .4738 and .8917, .4373 and .8938; here the speed was 7 or 8 times that of the optimum gradient method.

It seems impossible to say how the improvement would behave with larger n.

The irregular decrease of $f(x_k)$ was observed also by Stein [11] for the almost optimum methods ($\beta \doteq 0.9$). The gradient methods for $\beta \doteq 1$ are slow to converge because the sequence $\{x_k - A^{-1} b\}$ approaches periodicity. On the other hand, the strongly non-periodic character of our accelerated process and of the almost optimum process is, we believe, at the root of their success; the vectors $x_k - A^{-1}b$ are not permitted to settle down into a periodicity.

We have in Table 2 a few data which afford a comparison of the accelerated gradient process m = 8 with the almost optimum method $\beta = 0.9$. The comparison should be regarded as only tentative, since we have no idea how the speed of either process varies with the order of the matrices or other factors. For the matrix B_1, and start $x_0^{(3)}$, we find r(5,87) = .8204 for 87 steps of the almost optimum process ($\beta = 0.9$)*, while for the accelerated process (m = 8) we have r(5, 119) = .6245. For B_2, θ, and starts $x_0^{(6)}$, $x_0^{(7)}$, $x_0^{(8)}$, the comparable figures are: .6530 and .4566; .7117 and .4738; .6333 and .4373. If these figures are representative, the accelerated scheme (m = 8) is about twice as fast as the almost-optimum method ($\beta = 0.9$). On the other hand, the latter process surely requires

---

*For the similar matrix B_0, Stein's runs yield r(5,30) = .8065 (see Table 3); the irregularity of the process accounts for the discrepancy.

a simpler and shorter code - an exceedingly important advantage with machines.

In the straight runs with B_1 and B_2 of the optimum gradient method ($\beta = 1$) in Table 2 we have several samples of the ratio $r(s-1, s)$, which appears to be near its limit. According to (8), this ratio cannot exceed μ^2. Now

$$\text{for } B_0 \text{ and } B_1, \ \mu^2 = .97865832 \ ,$$

$$\text{for } B_2, \qquad \mu^2 = .89481373 \ .$$

We find that, of the six values of $r(s-1, s)$, all are greater than 99 per cent of their maximum value μ^2, while five exceed 99.6 per cent. This confirms the statement made in section II that Kantovorich's inequality (9) is close to an equality in practice.

In our one long run made with $\beta > 1$, we observe that $r(s-1, s) = .97865$, which agrees with μ^2 to five decimals. We also observe that, in Stein's four runs with $\beta > 1$, three of them have $r(s-1, s) = .9779$. We thus observe for $n = 6$ an apparent behavior of the modified gradient method ($1 < \beta < 2$) which is like that remarked in section II to be universally true for $n = 2$: for most x_0 and for β in a range $1 < \beta \leq \beta_0 < 2$, one has $f(x_k)/f(x_{k-1}) \to \mu^2$, as $k \to \infty$.

V. REFERENCES

[1] V. Bargmann, D. Montgomery, and J. von Neumann, "Solution of linear systems of high order," Report on Contract NORD-9596, prepared for the Bureau of Ordnance, U. S. Navy, 25 October 1946, Princeton, New Jersey.

[2] A. L. Cauchy, "Méthode générale pour la résolution des systèmes d'équations simultanées" Academie des Sciences, Paris, Comptes-Rendus, 25 (1847), 536-538.

[3] R. Courant and D. Hilbert, "Methoden der mathematischen Physik," Berlin, 1931.

[4] G. E. Forsythe and T. S. Motzkin, "Asymptotic properties of the optimum gradient method," American Mathematical Society, Bulletin, 57 (1951), 183 (Abstract).

[5] G. E. Forsythe and T. S. Motzkin, "Acceleration of the optimum gradient method. Preliminary report," American Mathematical Society, Bulletin, 57 (1951), 304-305 (Abstract).

[6] M. R. Hestenes and W. Karush, "A method of gradients for the calculation of the characteristic roots and vectors of a real symmetric matrix," National Bureau of Standards, Journal of Research, 47 (1951), 45-61.

[7] Magnus R. Hestenes and Marvin L. Stein, "The solution of linear equations by minimization," NAML Report 52-45, 12 December 1951, multilithed typescript, 35 pp.

[8] Magnus R. Hestenes and Eduard Stiefel, "Method of conjugate gradients for solving linear systems", NBS Report 1659, 10 March 1952, multilithed, 101 pp.

[9] L. V. Kantorovich, "Functional analysis and applied mathematics," Uspekhi matematicheskikh nauk, 3, no. 6 (1948), 89-185 (Russian).

[10] W. Karush, "An iterative method for finding characteristic vectors of a symmetric matrix," Pacific Journal of Mathematics, 1 (1951), 233-248.

[11] Marvin L. Stein, "Gradient methods in the solution of systems of linear equations," NAML Report 52-7, 20 July 1951, multilithed typescript, 18 pp.

[12] G. Temple, "The general theory of relaxation methods applied to linear systems," Royal Society of London, Proceedings, Series A, 169 (1939), 476-500.

THE NATIONAL BUREAU OF STANDARDS

Functions and Activities

The National Bureau of Standards is the principal agency of the Federal Government for fundamental and applied research in physics, mathematics, chemistry, and engineering. Its activities range from the determination of physical constants and properties of materials, the development and maintenance of the national standards of measurement in the physical sciences, and the development of methods and instruments of measurement, to the development of special devices for the military and civilian agencies of the Government. The work includes basic and applied research, development, engineering, instrumentation, testing, evaluation, calibration services, and various scientific and technical advisory services. A major portion of the NBS work is performed for other government agencies, particularly the Department of Defense and the Atomic Energy Commission. The functions of the National Bureau of Standards are set forth in the Act of Congress, March 3, 1901, as amended by Congress in Public Law 619, 1950. The scope of activities is suggested in the listing of divisions and sections on the inside of the front cover.

Reports and Publications

The results of the Bureau's work take the form of either actual equipment and devices or published papers and reports. Reports are issued to the sponsoring agency of a particular project or program. Published papers appear either in the Bureau's own series of publications or in the journals of professional and scientific societies. The Bureau itself publishes three monthly periodicals, available from the Government Printing Office: the Journal of Research, which presents complete papers reporting technical investigations; the Technical News Bulletin, which presents summary and preliminary reports on work in progress; and Basic Radio Propagation Predictions, which provides data for determining the best frequencies to use for radio communications throughout the world. There are also five series of nonperiodical publications: the Applied Mathematics Series, Circulars, Handbooks, Building Materials and Structures Reports, and Miscellaneous Publications.

Information on the Bureau's publications can be found in NBS Circular 460, Publications of the National Bureau of Standards ($1.00). Information on calibration services and fees can be found in NBS Circular 483, Testing by the National Bureau of Standards (25 cents). Both are available from the Government Printing Office. Inquiries regarding the Bureau's reports and publications should be addressed to the Office of Scientific Publications, National Bureau of Standards, Washington 25, D. C.

NBS